

frac. valid SMILES

1.0  
0.5

frac. unique SMILES

1.0  
0.5

frac. SMILES in train

0.05  
0.00  
-0.05

frac. SMILES in PubChem

1.00  
0.95

KLD  
0.75  
0.50

Frechet distance

50  
25

frac. SMILES with azo

1  
0

SA score

3.5  
3.0

0.0 0.5 1.0 1.5 2.0  
temperature

